Propane Oxidation at High Pressure and Intermediate Temperatures

Hashemi, Hamid; Christensen, Jakob Munkholt; Glarborg, Peter

Publication date:
2016

Document Version
Peer reviewed version

Propane Oxidation at High Pressure and Intermediate Temperatures

Hamid Hashemi, Jakob M. Christensen, Peter Glarborg

Department of Chemical Engineering, Technical University of Denmark (DTU), DK-2800 Kgs. Lyngby, Denmark

Email: pgl@kt.dtu.dk (P. Glarborg)

hah@kt.dtu.dk (H. Hashemi)

36TH International Symposium on Combustion
COEX, SEOUL, KOREA July 31 - August 5, 2016

Technical University of Denmark

Experimental: Laminar Flow Reactor (FR)

- Quartz reactor to minimize surface reactions
- Steel pressure shell to achieve high pressures
- Temperature: 500–900 K
- Pressure: 100 bar
- Isothermal Zone Length: 42–44 cm
- Residence time: 8—11 s
- Measurement via GC and Gas Analyzer

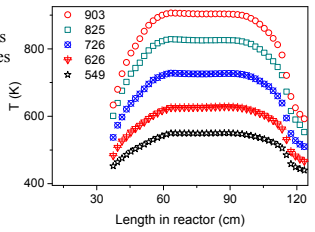

Fig 1. Temperature profile measured inside the pressure-shell wall of the reactor

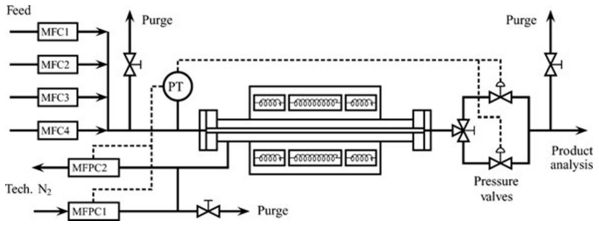

Fig 2. Schematic diagram of the high pressure laminar flow reactor

Chemical Kinetics Model

- H_2/CO/HC's subsets from recent work by Glarborg et al. [1—3].
- C_3 subset is reviewed and introduced in *p.w.*
- Low temperature sequences for propane oxidation is adopted from Goldsmith et al. [4].

Results: Flow Reactor (FR)

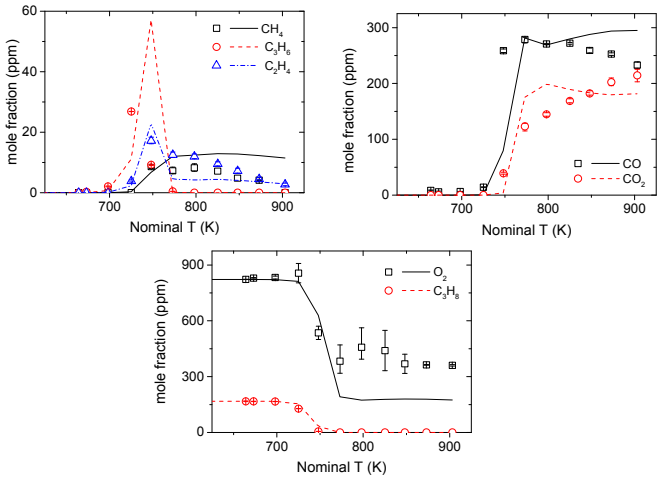

Fig 3. Experiments in the flow reactor at 100 bar pressure. The initial conditions were 168/ 822 ppm of C_3H_8/O_2 in N_2 (Φ=1). Residence time varies between 8 and 11 s.

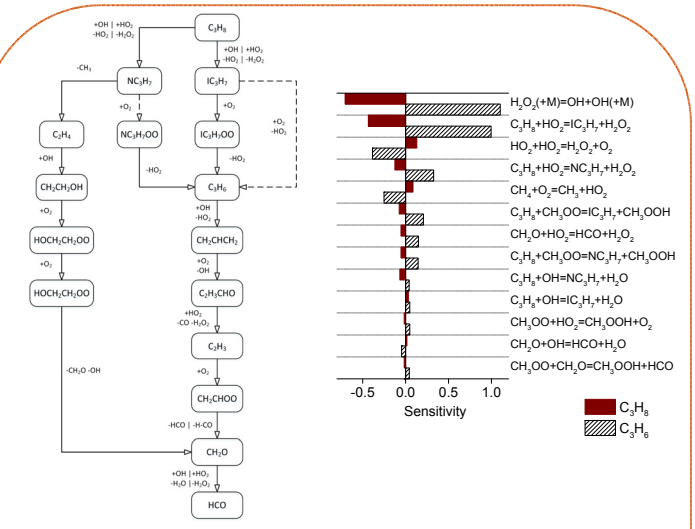

Fig 4. ***Left:*** Reaction pathways of propane oxidation at conditions investigated in the flow reactor (100 bar, 750 K). ***Right:*** Sensitivity of C_3H_8 and C_3H_6 prediction under flow-reactor conditions (100 bar, 750 K).

Results: Comparing the Model with Literature

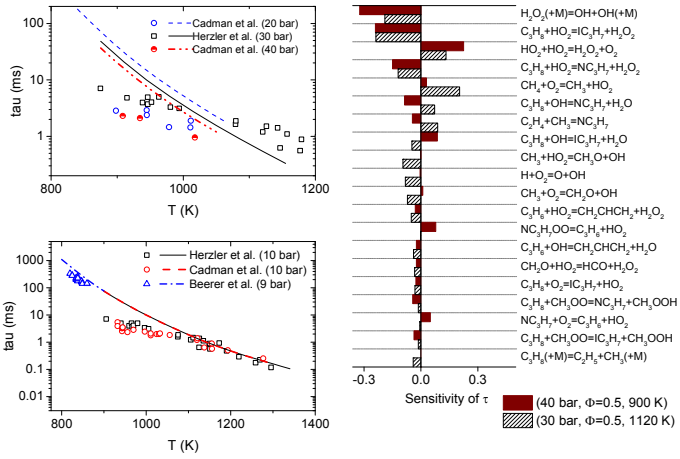

Fig 5. ***Left:*** Ignition delay times of propane. The experiments are from Herzler et al. [5] and Cadman et al. [6] (2.1% C_3H_8 + 20.6% O_2 in N_2, Φ=0.5), and Beerer et al. [7] (2.5% C_3H_8 + 20.5% O_2 in N_2, Φ=0.6). ***Right:*** Sensitivity of ignition delay time of propane to reaction rate constants (2.1% C_3H_8 + 20.6% O_2 in N_2 , Φ=0.5).

Summary & Future Work

- Propane oxidation in the flow reactor:
  - — Onset at 725—750 K (100 bar, Φ=1)
  - — Accurate model prediction
  - — Importance of abstraction reaction C_3H_8+ HO_2
- The model prediction of ignition delay times:
  - — Over-prediction at intermediate T (900—1000 K)
  - — Inaccuracy in transition from low-T to high-T regimes
- Further experiments on propane oxidation at different P and Φ are planned.
- Further work is required to improve the model prediction, especially for ignition delays.

References

[1] H. Hashemi, J. M. Christensen, S. Gersen, P. Glarborg, "Hydrogen oxidation at high pressure and intermediate temperatures: Experiments and kinetic modeling", Proc. Combust. Inst. 35 (2015) 553–560.

[2] H. Hashemi, J. M. Christensen, S. Gersen, H.B. Levinsky, S.J. Klippenstein, P. Glarborg, "High-pressure oxidation of methane", Combust. Flame (accepted), 2016.

[3] J. Lopez, C. Rasmussen, H. Hashemi, M. Alzueta, Y. Gao, P. Marshall, C. Goldsmith, P. Glarborg, "Experimental and kinetic modeling study of C_2H_2 oxidation at high pressure", Int. J. Chem. Kinet. (accepted), 2016.

[4] C. F. Goldsmith, W. H. Green, S. J. Klippenstein, "Role of O_2 + QOOH in low-temperature ignition of propane. 1. Temperature and pressure dependent rate coefficients", J. Phys. Chem. A 116 (2012) 3325–3346.

[5] J. Herzler, L. Jerig, P. Roth, "Shock-tube study of the ignition of propane at intermediate temperatures and high pressures", Combust. Sci. Technol. 176 (2004) 1627–1637.

[6] P. Cadman, G. O. Thomas, P. Butler, "The auto-ignition of propane at intermediate temperatures and high pressures", Phys. Chem. Chem. Phys. 2 (2000) 5411–5419.

[7] D. Beerer, V. McDonell, S. Samuelsen, L. Angello, "An experimental ignition delay study of alkane mixtures in turbulent flows at elevated pressures and intermediate temperatures", J. Eng. Gas Turbines Power 133 (2011) 011502.